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D6.1 DIMAT SIMULATION AND OPTIMIZATION SUITE

14/03/2025

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D6.1 DIMAT SIMULATION AND OPTIMISATION SUITE

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Abstract	The present document, titled Simulation and Optimization Suite version 2 (D6.1), unveils the innovative strides made in the first 18 months of the project. It provides technical information regarding the development activities for building the cutting-edge digital technologies described in WP6. It details the principal features, technical specification, implementation status, and the next steps in developing and implementing each toolkit that composes Simulation and Optimization Suite, a set of toolkits for predicting material mechanical behaviour, creating efficient materials manufacturing simulation processes, and providing modular tools that can support interactions with physical equipment.
Keywords	MECHANICAL PROPERTIES SIMULATOR, MATERIALS PROCESSING SIMULATOR, DIGITAL TWIN, PROCESS CONTROL, PREDICTION, NUMERICAL MODEL, MECHANICAL MODEL, PYTHON ENVIRONMENT, AUTOMATIZATION, MODELING WORKFLOW

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Document Revision History

Version	Date	Description of change	List of contributor(s)
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EXECUTIVE SUMMARY

The present document, titled Simulation and Optimisation Suite version 2 (D6.1), unveils the innovative strides made in the first 18 months of the project. It provides technical information regarding the development activities for building the cutting-edge digital technologies described in WP6. It details the principal features, technical specification, implementation status, and the upcoming steps in the enhancement and implementation of each toolkit that composes the Simulation and Optimisation Suite, a set of toolkits for predicting material mechanical behaviour, creating efficient materials manufacturing simulation processes, and providing modular tools that can support interactions with physical equipment.

Specifically, this document provides detailed information related to the mechanical and numerical model design used as the basis for pilot case solutions and the combination of different numerical freeware codes that led to the development of the following three toolkits:

The Materials Mechanical Simulator (Di^{MMS}) is a toolkit created to forecast the mechanical properties of materials and components based on their composition, structure, and configuration.

The DiMAT Materials Processing Simulator (Di^{MPS}) is a digital toolkit designed to recreate manufacturing processes to predict materials' behaviour when modifying the process condition and material properties.

The Digital Twin for Process Control (Di^{DTPC}) toolkit is a practical solution that provides a set of digital twins of the devices considered for the Pilot use cases. These digital twins are not just theoretical models but modular tools that can support interactions with physical equipment. The DTPC toolkit offers access to functionalities that enable the efficient monitoring of the manufacturing operations carried out by the “twinned” devices and access to simulation algorithms through its connection with the rest of the toolkits of this suite.

This deliverable is an updated version that addresses all comments provided by the reviewer and the Project Officer. To ensure clarity and transparency, we have created a detailed table summarizing the changes made to this document in response to the reviewer's feedback. The Table 2 can be found in the appendix, providing an overview of the revisions and additions for easy reference.

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ABBREVIATIONS

AI	Artificial Intelligence
API	Application Programming Interface
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
cVO	Composite Virtual Object
D	Deliverable
DT	Digital Twin
EMMC	European Material Modelling Council
FEA	Finite Element Analysis
FOAM	Focus on Opportunity, Ability and Motivation
FRD	Functional Requirements Document
HTTP	Hypertext Transfer Protocol.
IoT	Internet of Things.
KAF	Knowledge Acquisition Framework
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
MODA	Modelling Data
PCA	Principal Component Analysis
POD-RBF	Proper Orthogonal Decomposition with Radial Basis Functions
RBF	Radial Basis Function
STEP	Standard for the Exchange of Project Data
T	Task
TCP	Transmission Control Protocol
VO	Virtual Object

XAI	Explainable Artificial Intelligence

DiMAT Toolkits

CMDB	Cloud Materials Database
KAF	Knowledge Acquisition Framework
MEC-LCA	Materials Environmental and Cost Life Cycle Assessment
MDF	Materials Design Framework
MM	Materials Modeler
MD	Materials Designer
MMS	Materials Mechanical Properties Simulator
MPS	Materials Processing Simulator
DTPC	Digital Twin for Process Control

1 DIMAT MATERIALS MECHANICAL PROPERTIES SIMULATOR – DI^{MMS}

1.1 OVERVIEW

The DiMAT Materials Mechanical Properties Simulator (Di^{MMS}) is a comprehensive numerical toolkit designed to accurately predict the mechanical properties of materials based on their composition, structure, and configuration. These properties encompass stiffness, strength, damage, fracture, and rheological properties such as creep and viscoelastic and viscoelastic behaviour.

The MMS toolkit is aligned with the objectives of the DiMAT project, with O6 and O6.1. Utilizing a combination of Finite Element Analysis (FEA), atomistic codes, and data-driven models, the toolkit operates across multiple scales, including micro-, meso-, and macroscopic levels.

1.2 FEATURES

The mechanical model connects input variables, including dimensional specifications and material properties, to the resulting output (the mechanical performance). This toolkit streamlines material and product design processes, optimising their efficiency and performance.

The mechanical model follows the requirements defined by EMMC (European Material Modelling Council) in **MODA**, a template for the standardized description of materials models. The MODA provides all necessary aspects for description, reproducibility, and interfacing with other models. MODA provides a structured format for documenting all model parameters, assumptions, inputs, and outputs involved in defining mechanical material behaviours.

A **hierarchical multiscale approach** is employed to link macro-mechanical properties with microstructure and constitutive equations of materials and components. The multiscale simulation is then complemented by Multiphysics models and artificial intelligence.

The MMS toolkit is developed with open-source software (e.g., Calculix, LAMMPS), ensuring accessibility and flexibility. These elements will be customized to suit specific user needs and seamlessly integrated into a **user-friendly** interface.

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Additionally, the interface prioritizes intuitive design, fostering a more productive user experience. MMS provides the possibility for **real-time** operation. In this sense, a reduced or surrogate model based on machine learning algorithms is developed to deliver a quick response akin to the physical models.

1.3 TECHNICAL SPECIFICATIONS

The backend of the MMS toolkit will be developed by combining different numerical freeware codes:

- Molecular dynamic codes: LAMMPS
- Finite element codes: GMSH, CALCULIX, PrePoMax,
- Auxiliary elements: LSDYNA LS-Prepost, FreeCad, PYTHON

Molecular dynamics simulations will be conducted using LAMMPS, with automation handled by PYTHON. Finite element simulations are divided into preprocessing, solving, and post-processing. The preprocessing tasks have been realized with GMSH and LS-Prepost, the solver employed is CALCULIX, and post-processing tasks are performed with PrePoMax. Automation scripts are written in Python, utilizing essential libraries such as NumPy, SciPy, Matplotlib, and Pandas. The simulations obtained from the combination of atomistic and finite elements results will be integrated into a surrogate model using machine learning and AI algorithms, which will be displayed through the front-end.

1.4 IMPLEMENTATION STATUS

1.4.1 Current Implementation

The current implementation of Di^{MMS} includes the following features:

- Development of a finite element model for the fishing net of TECNORED, linking net dimensions with stress and stress concentration ratio. Contact-rich textile structures, such as the fishing nets used by TECNORED, present significant challenges for finite element simulations due to the multitude of contact interfaces. Traditional 3D continuum approaches become computationally prohibitive when each filament must be discretized and contact constraints tracked from uncertain initial configurations. DiMAT methodology integrates discrete particle simulations, employing software such as LAMMPS, with continuum-based FE analysis tailored explicitly to TECNORED fishing nets. Each filament within the net is initially represented as a discrete particle chain. This particle-based model accurately captures axial and bending stiffness, along with frictional contact. This allows the system to rapidly converge to an equilibrium arrangement. Upon achieving equilibrium, filament geometries are exported into a Finite Element framework, where a two-step simulation is conducted. The first step involves a preliminary tying analysis. The second step involves a fully coupled FE analysis that applies mechanical loads.

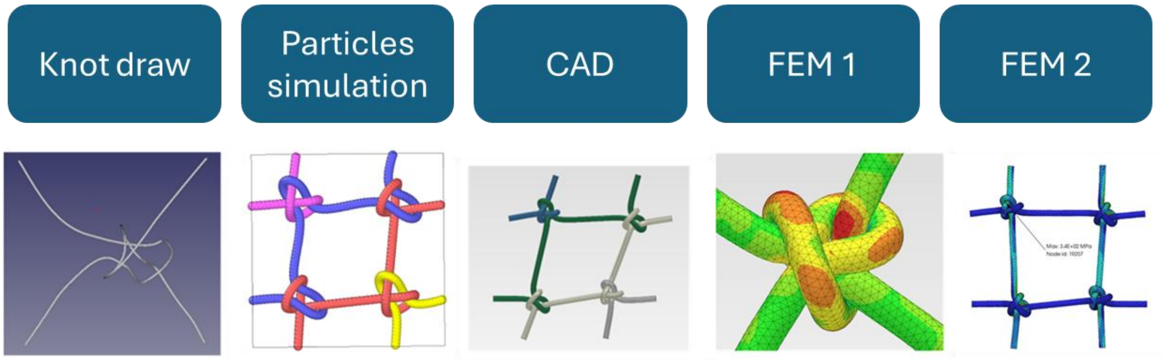

Figure 1: Complex modelling workflows in PL1-TECNORED: NET.

- The previous multistep workflow has been integrated into a machine learning-based subrogated model. This reduced model has been trained on real simulation data, enabling real-time predictions and significantly reducing computation time while maintaining high accuracy. The basic idea is to develop a model miming the physical input-output relationship. The model leverages Principal Component Analysis (PCA) in conjunction with Radial Basis Function (RBF) interpolation to relate input parameters directly to mechanical performance outcomes. The surrogate model functions as a digital replica of the physical system and exemplifies a practical application of Explainable Artificial Intelligence (XAI). Within this framework, the machine learning model closely approximates the behaviour of the physical system, while the underlying physics-based model provides interpretability and validation. If needed, predictions from the surrogate model can be explained and verified by referencing the original physics-based simulations, enhancing confidence in the reliability and interpretability of the model. The reduced model has been used as the core of the toolkit backend.
- Implementation of Keycloak in the frontend to ensure secure access to the toolkit. Results from all analyzed cases are saved and accessible from the home page. New simulations can be initiated, with the input being the dimensions of the fishing net and the output being the maximum stress field and stress ratio. Additionally, a 3D graphical output has been incorporated to visualize stress contours.
- The application of the MMS toolkit to the NET TECNORED model for the polymer pilot meets the requirements of T2.3.

The toolkit is deployed and accessible for users at the following link: https://mms.dimat-tools.eu/
Link to the Demo version of the solution:

https://youtu.be/yzfAwCYMrhs

1.4.2 Next developments

The future development and implementation of Di^{MMS} will include the following (prioritized to pilots' needs):

- In PL1, the toolkit will be applied to NATURPLAST and AITEX to develop a comprehensive multiscale polymer model, analyzing the compound composition, spinning process, braiding techniques, and the resulting mechanical performance.
- Enhancement of the 3D contours included in the graphical interface.
- Incorporation of graphical elements in the input section, enabling visualization of geometry or component fraction modifications.
- Introduction of optimization capabilities. The toolkit will incorporate parametric simulation capabilities, enabling users to define specific constraints and objective functions.
- Extension of MMS input-output application to fulfil all pilot requirements related to the toolkit.

The real-time mode currently implemented provides quick predictions through surrogate models but requires extensive retraining for each new scenario involving different materials, geometries, or structural modifications. A new server mode will be introduced to address these limitations and offer greater flexibility. This server mode allows users to perform comprehensive simulations directly without the constraints of retraining surrogate models, thus providing broader options and greater adaptability to changing customer requirements.

The MMS toolkit will ensure full compatibility and interoperability with open-source software. The toolkit will generate input/output files compatible with both atomistic and finite element open-source tools such as LAMMPS, CalculiX, FreeCAD, PrePoMax, OVITO, and ParaView. This compatibility will facilitate transparency and reproducibility, aligning the toolkit with open science principles.

The integration of MMS with other toolkits, such as CMDB, will be further developed. This will allow the retrieval of material data directly from the CMDB and the storage of numerical outputs for reuse in future simulations, enhancing data continuity and efficiency.

All features are expected to be implemented by the next release of the Suite.

2 DIMAT MATERIALS PROCESSING SIMULATOR – DI^{MPS}

2.1 OVERVIEW

The DiMAT Materials Processing Simulator (Di^{MPS}) is a digital toolkit designed to recreate manufacturing processes to predict materials' behaviour when modifying the process parameters. The simulation variables (temperature, pressure, time, etc.) are connected to the different requirements of the selected process, offering the opportunity to test a specific set of parameters by computer-aided design (CAD) geometries and numerical models, thus voiding direct interference with the production line in situ. The other variables are related to materials' properties and behaviour during their transformation, offering versatility to users when developing a study and introducing new materials in manufacturing.

Di^{MPS} toolkit provides a digital interface with 3D graphical contours to allow the simulation results to be analyzed. The simulation of materials processing is generated by specific CAD geometry and boundary conditions using finite element Analysis (FEA) and computational fluid dynamics (CFD). The generated results are stored for further processing and develop accurate simulations. The data storage is further used to interact with the other DiMAT toolkits, developing a common materials library for a better comprehensive material study.

The Di^{MPS} toolkit is aligned with the objectives of the DiMAT project on the development of simulation and optimization suites WP6 and T6.2. This task aims to implement Explainable Artificial Intelligence (XAI) techniques to accurately predict manufacturing processes' behaviour. These specific XAI techniques are based on implementing surrogate models using interpolation, data reduction, and machine learning techniques to replace complex simulations. The surrogate model facilitates workflow automation, allowing any software or user to run the model easily.

The Di^{MPS} toolkit is designed to be able to interact with the learning systems of the neural networks (deep learning). Once the AI network algorithm has been generated, the training must be applied to each one of the materials, processes, and processing conditions of the existing database to generate the desired knowledge.

2.2 FEATURES

Di^{MPS} toolkit is developed based on freeware such as FreeCAD, PrePoMax, Calculix, and OpenFoam, but not only. These components provide a dependable pathway for predicting materials behaviour under specific processing conditions, which can be replicated, adjusted, and tailored as per requirements.

For the pilot glass, the Di^{MPS} toolkit works on predicting the plastic deformation of a specific geometry, designed in FreeCad, which has included a parametrization function for dimensional specification. The simulation emulates the bending process of a glass sheet when heated above the so-called glass transition temperature (T_g), at which point the glass becomes soft and can be shaped into a convex or concave piece due to gravity. Starting from the designed geometry, a calculation and simulation of a viscoelastic deformation have been applied. The input variables are temperature degree, dimensional specification, and material properties such as viscosity against temperature, density, thermal expansion coefficient, etc., which lead to the resulting outputs (deformation degree and stress).

In the case of the pilot composite, the Di^{MPS} toolkit is focused on the curing resin degree. To this aim, a specific resin has been simulated on a mould of fixed geometry, in which the thermal and chemical properties of the resin have been incorporated. As a result, obtaining the degree and time of curing based on temperature.

Regarding pilot polymer, the Di^{MPS} toolkit intends to simulate a filament extrusion, in which, depending on specific properties of the material, such as density and viscosity, the extrusion conditions of the filament are determined in terms of variation in dimensions and temperature.

2.3 TECHNICAL SPECIFICATIONS

The backend of the Di^{MPS} toolkit is developed by combining different numerical freeware codes:

- Computational fluid dynamics codes: OpenFOAM
- Finite element codes: GMESH, CALCULIX, PrePoMax,
- Auxiliary elements: Salome, LS-Prepost, FreeCAD, PYTHON

For pilot glass, the calculation has been based on a simple geometry provided by the pilot partner, implementing a viscoelastic model. The calculations have been done using the PrePomax program with the auxiliary elements of Calculix as the default solver, allowing multiple simulations to be carried out under different conditions.

In the second stage, a set of solutions is listed as the result of the simulations carried out under specific conditions. Subsequently, two algorithms have been programmed: automation and multivariable interpolation of predefined calculations.

The automated process herein is applicable for all pilots; it begins with the CAD file collection saved in (*.stp)* format, each containing the solid bodies placed at the final assembly configuration of the problem. The simulation output is provided in CALCULIX output file (*.frd*) format, containing data on mechanical displacements, temperatures, strains, and stresses.

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A PYTHON function capable of converting STEP files into FRD files has been developed to facilitate this automation. Furthermore, another function has been created to parse FRD files and import their data into the PYTHON environment for subsequent analysis. The operational workflow of this process is illustrated in Figure 2.

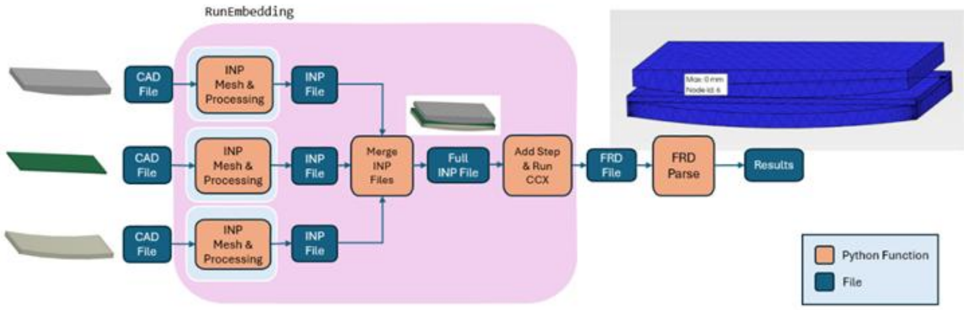

Figure 2: Example of Automatization modeling workflow.

For the pilot Composite, the simulation calculations were based on fixed geometry using the OpenFOAM framework. The starting point for the curing resin simulation has been the *laplacianFoam* solver, which can solve the unsteady heat transfer equation in solids. The code of the *laplacianFoam* solver has been modified for the pilot partner, adding the source term in the heat equation and the evolution equation of the degree of cure as the new field **alpha**.

The modified solver has been compiled with the provisional name of *dimatFoam* and can be used within the OpenFOAM framework. This solver has been tested and validated using experimental data from a real case scenario, resulting in a coincidence of more than 97% in the values obtained.

In the case of the pilot polymer, the simulation was implemented by creating a fixed geometry in FreeCAD based on a cylinder that emulates the filament outlet from the extruder head. The extrusion simulation has been generated using OpenFoam. It should be noted that OpenFoam is incorporated into Freecad as a plugin. Then, the dimensional variations of the extruded filament and temperature variants are obtained.

2.4 IMPLEMENTATION STATUS

2.4.1 Current Implementation

The current implementation of Di^{MPS} includes the following:

The finite element model for the glass bending process of the HEGLA pilot has been developed, linking the input variables and a viscoelastic model with the glass sheet deformation degree and stress. This solution has been integrated into a subrogated model serving as the core of the backend.

The surrogate model is based on the POD-RBF (Proper Orthogonal Decomposition with Radial Basis Functions) procedure to approximate the results of CFD simulations performed with OpenFOAM. Its purpose is to reduce the computational cost of simulations, allowing for fast predictions of key variables based on input parameters. The current implementation also includes the first version of a fronted development. This front-end provides an intuitive user interface, with a set of options that allow modelling the glass-bending process by having the processing temperature as input. Figure 3, Figure 4 and Figure 5 show the initial view of the MPS toolkit, an example of the MPS numerical input and the MPS numerical output, respectively.

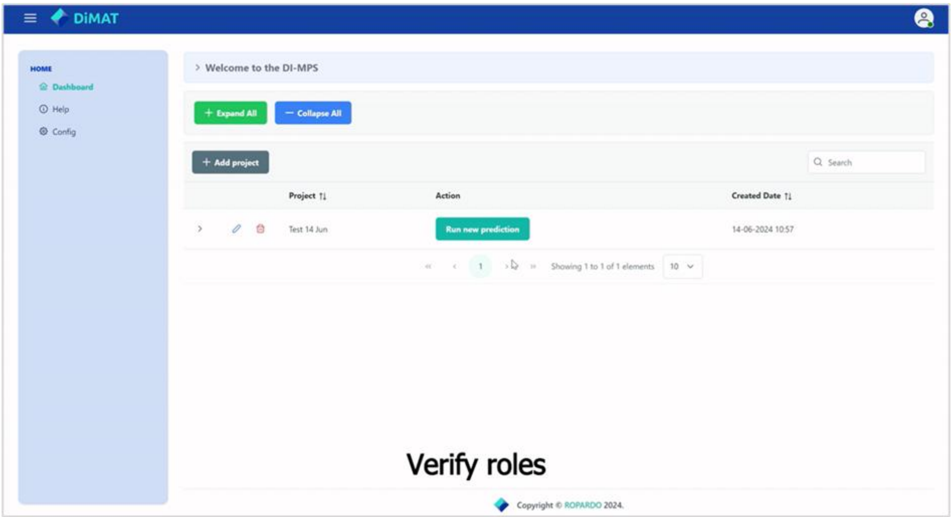

Figure 3: Initial view of the MPS toolkit.

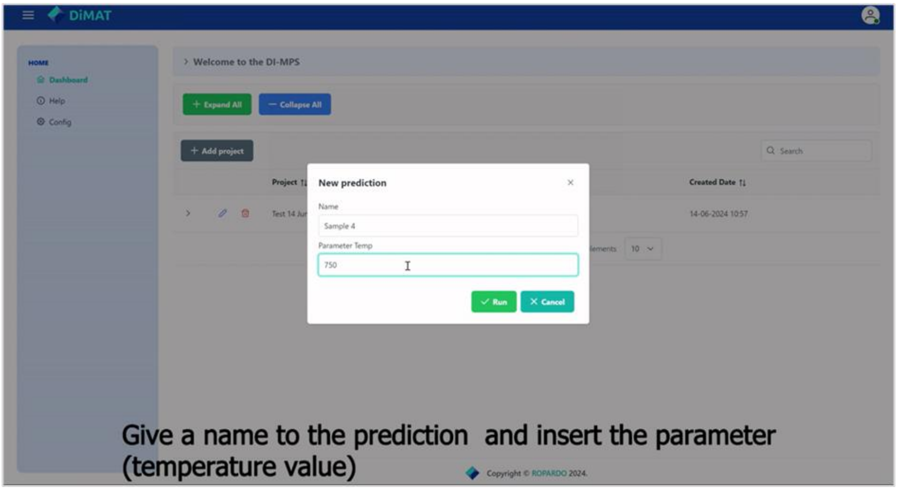

Figure 4: Example of the MPS numerical input.

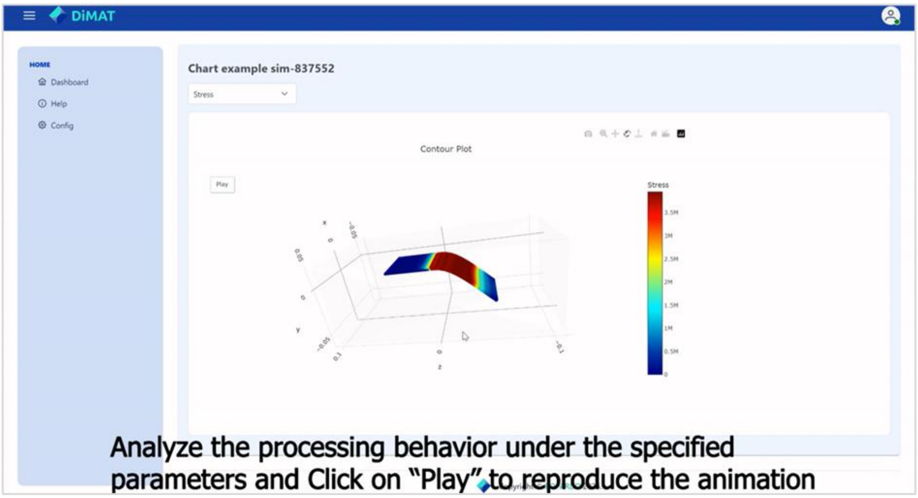

Figure 5: Example of the MPS numerical output.

- Keycloak implementation in the toolkit front-end. Results from all analyzed cases are saved and accessible from the initial page. New simulations can be initiated, with the input being the initial processing temperature and materials properties. As output, being the deformation degree and stress. In addition, a 3D graphical output has been incorporated to visualize deformation degree and stress contours.
- The finite element model for the curing resin prediction of the CETMA pilot has been developed, integrating the new dimatFoam solver in the framework of OpeanFoam. This solver has been developed by the pilot partner, aiming to enhance the accuracy of the curing resin simulation. At this stage, several simulations of curing resin are being carried

out by varying the curing parameters, aiming to collect the corresponding data for automating the modeling tasks (get into the backend development).

- The finite element model for the melt spinning process for the AITEX polymer pilot has been developed.

The toolkit is deployed and accessible for users at the following link: https://mps.dimat-tools.eu/

Link to the Demo video of the solution:

https://www.youtube.com/watch?v=JXr2Y8hLMGs

2.4.2 Next developments

The future development and implementation of DiMPS will include the following (prioritized to pilots' needs):

1. Optimization of the features implemented for the pilot glass simulation.
   1.1. Improve the existing subrogate model to develop an enhanced and updated backend and frontend.
2. Implementing curing resin prediction for CETMA composite into the front-end of the DiMPS toolkit.
   2.1. Study the feasibility of using various preprocessors, such as Salome or FreeCad, for the pilot composite solution.
   2.2. Evaluate the feasibility of incorporating more complex geometry in the simulation of the curing resin.
3. Implementing the melt spinning process for the AITEX polymer pilot into the front-end of the DiMPS toolkit.
   3.1. Thermal and Structural Models development for melt spinning process simulation.
4. Implementing the polymer extrusion for the NATUREPLAST polymer pilot into the front-end of the DiMPS toolkit.
   4.1. Thermo-mechanical model development for the polymer extrusion process simulation.
   4.2. Database creation from processing parameters using Python routine.

The above mentioned activities will be carried out according to the following time plan:

		The month of the project				
Activity		20	21	22	23	24
1						
1.1						
2						
2.1						
2,2						
3						
3.1						
4						
4.1						
4.2						

Table 1: Time plan for the MPS toolkit's next developments.

To allocate these activities in a logical sequence over five months until the next deliverable, priorities were considered based on the degree of complexity of their execution and considering activities with significant progress. Therefore, the less complex activities were placed to be carried out before the more complex ones. Also, activities with significant progress were allocated before activities with less progress. All features are expected to be implemented by the next release of the Suite.

3 DIMAT DIGITAL TWIN FOR PROCESS CONTROL – DI^{DTPC}

3.1 OVERVIEW

The Digital Twin for Process Control (DI^{DTPC}) toolkit provides a set of digital twins (DTs) that act as abstractions of the Internet-of-Things (IoT) devices that are involved in this Suite. It provides a means to monitor the processes in which the devices take part while also offering access to simulation and emulation algorithms. The design of the DTs is modular, secure, and easily deplorable. The DTs communicate with their physical counterparts and can also offer controlling functionalities. Their development is done using exclusively open-source software.

The progress in developing the DTPC toolkit aligns with the objectives and milestones of the DiMAT project. The first release of the toolkit contains functionalities that can be used by any pilot, as well as some more specific functionalities tailored to the particular pilot use cases.

3.2 FEATURES

The DTPC supports the following features:

- Monitoring of processes: The deployed DTs gather time-series data from the IoT devices deployed at the customer's side and use them as input to functionalities that have been developed to ensure the correct operation of the machinery.
- Communication/control of IoT devices: The DT can communicate with the physical counterparts (IoT devices) and issue commands when necessary.
- Time-series forecasting: A set of forecasting techniques for time-series data is provided so that the user can select and set parameters (default parameters offered but can be modified) and see visualizations of the estimated values for the time-series data.
- Alerts: The user can set customized alerts indicating the appropriate ranges for the metrics measured by the Virtual Objects.
- Dashboards: Dashboards showing useful information are provided. The user can select to change the default metrics presented.
- Visualizations: Access to visualizations regarding the process monitored by each DT.

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3.3 TECHNICAL SPECIFICATIONS

Technologies:

- The developed DTs are based on the Nephele Virtual Object (VO) Software Stack (open source)
- Forecasting algorithms are implemented with Prophet. ARIMA and Machine learning models from Python libraries
- The code used for the virtual functions defined in each VO is developed in Python.
- The code used for visualizing 3D objects was developed using the Mayavi Python library.
- 2D visualizations (graphs, surface plots) are generated using the Plotly library,
- The database used for storing time-series data was InfluxDB
- The front-end of the application is developed with Vue.js
- The back-end services are implemented using Flask API (Python)) and Node.js (Javascript)

The VOs can support different virtual functions according to the corresponding process or equipment that they “twin”. The VOs are usually deployed at the edge of the infrastructure and exchange data with Internet-of-Things (IoT) devices. They can communicate with each other over public HTTP Restful APIs. This ensures the scalability of the solution as well as the microservices approach on which the DTPC toolkit can be deployed since a change in the Virtual Function of a VO does not affect the operation of the other deployed (c)VOs.

The solution is provided to the customers/users as a Docker image. The necessary computing resources vary on the complexity of the developed virtual functions for each Digital Twin. The DTs can be deployed on the network edge if they are lightweight or on servers if more computing power is required.

3.4 IMPLEMENTATION STATUS

3.4.1 Current Implementation

At this stage, a first version of the implementation of the DTPC is available, focusing on the following features:

- Capability of setting alerts for devices that produce time-series data through the user interface. (Figure 6)
- Forecasting using Prophet, ARIMA, AutoARIMA, and LSTM models. (Figure 7)

- Dashboards for time-series data evolution inspection (Figure 8)
- Visualization of temperature distribution inside a furnace used for glass bending for Glass Pilot (Figure 9)
- Monitoring of the data measured by data loggers of the Composite Pilot and generating alerts based on defined conditions by the Pilot.
- Secure access to the toolkit using Keycloak. (Figure 10)

Following, we provide some indicative screenshots from the current version of the DTPC.

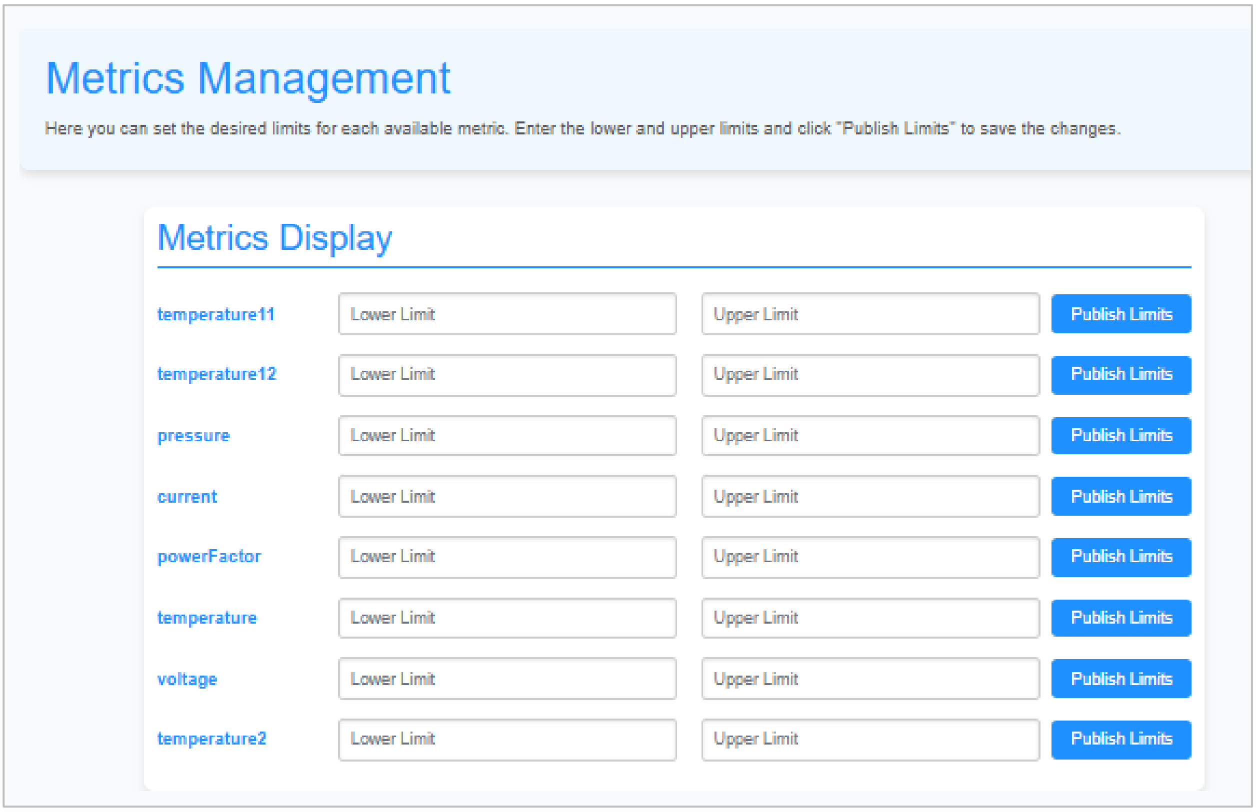

Figure 6: Setting custom metric limits to produce the corresponding alerts (DTPC toolkit).

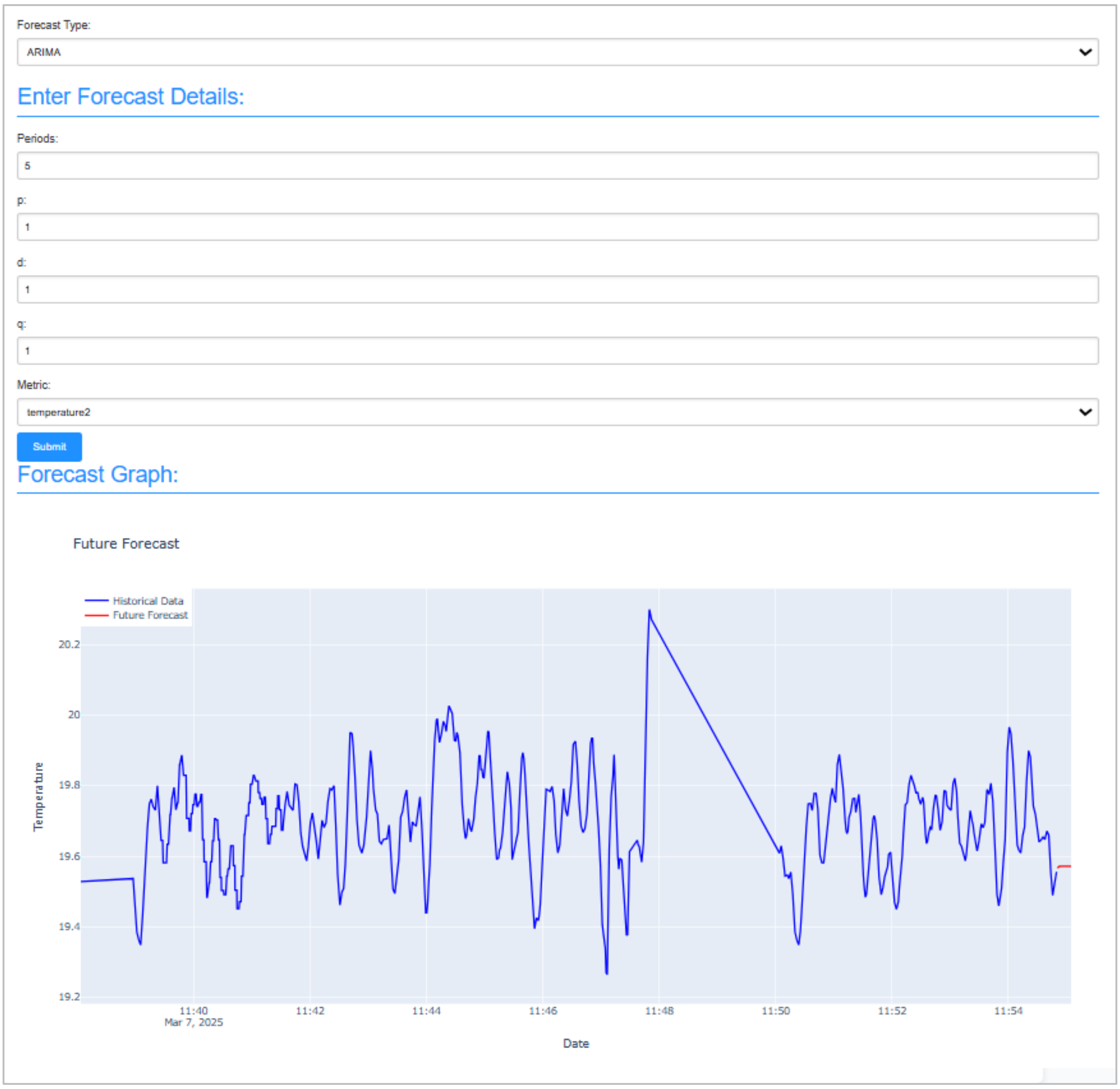

Figure 7: Example of Arima forecasting for the temperature metric DTPC toolkit.

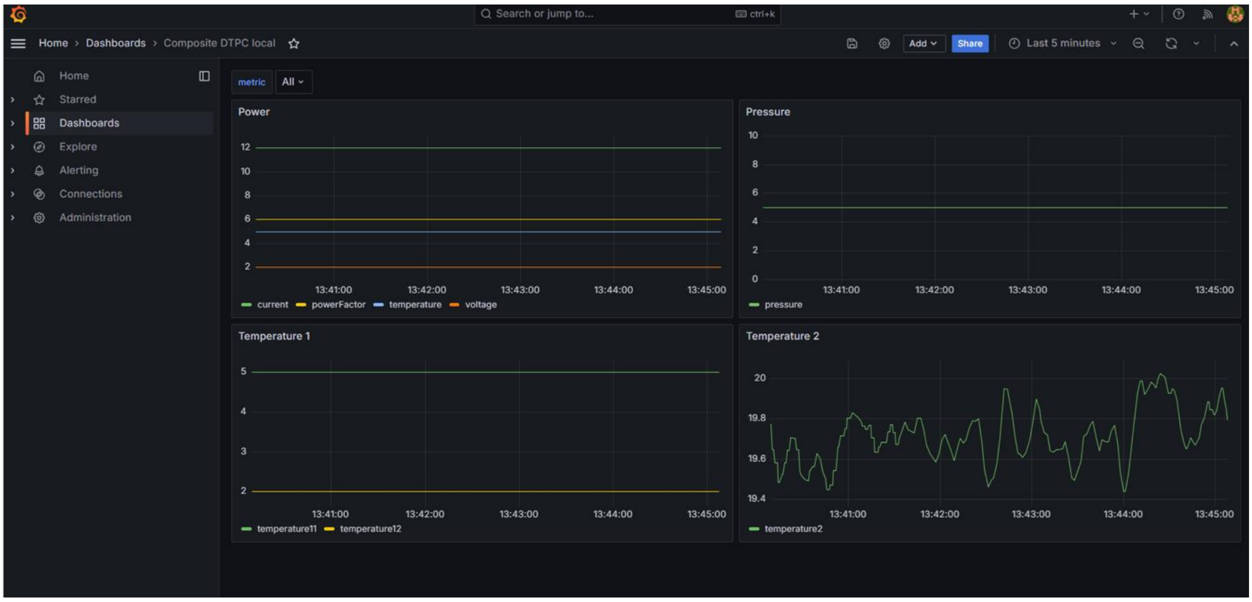

Figure 8: Dashboard for time series data evolution (DTPC toolkit).

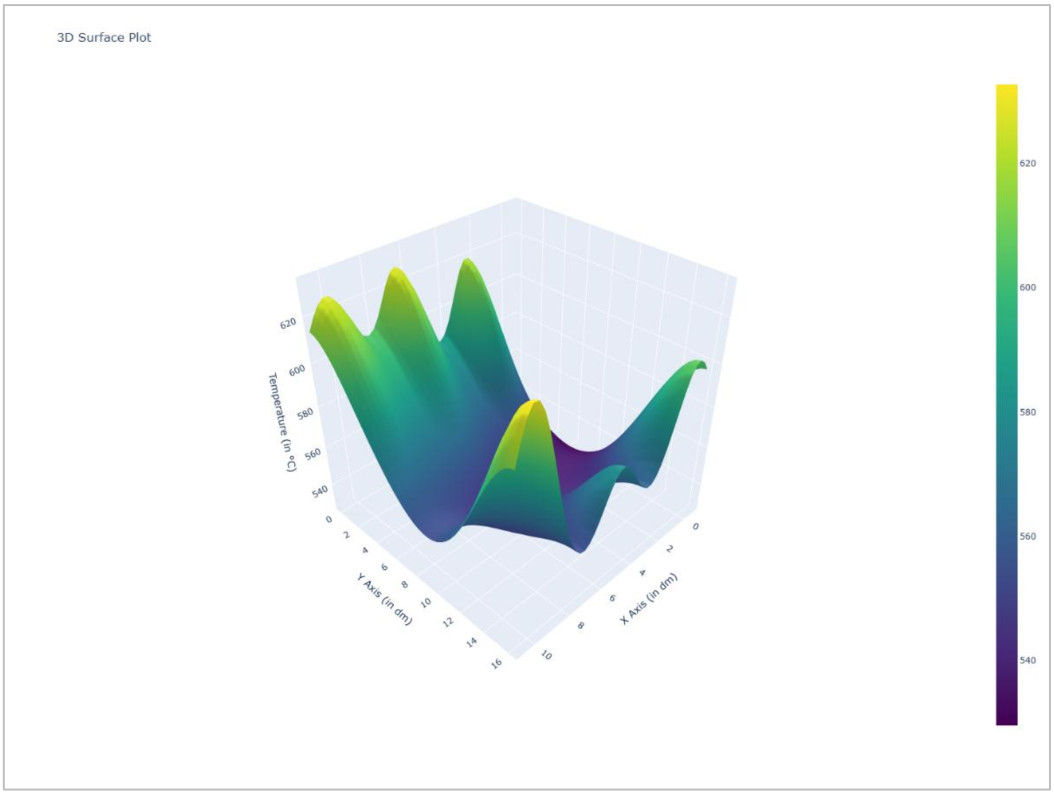

Figure 9: Visualization of temperature distribution inside a furnace.

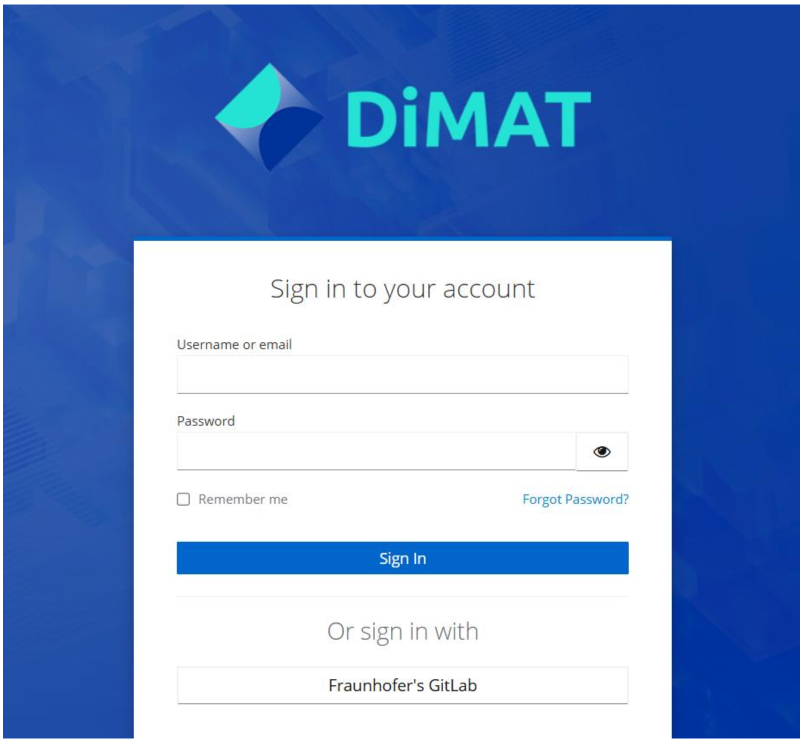

Figure 10: Secure access to the DTPC toolkit using keyloack.

Link to the GitLab repository of the solution:

https://gitlab.cc-asp.fraunhofer.de/dimat/simulation-and-optimisation-suite/digital-twin-for-process-control/dtpc

Link to demo video:

https://www.youtube.com/watch?v=WDq12A3TqK0&t=63s&ab_channel=DiMAT

3.4.2 Next developments

The future development and implementation of Di^{DTPC} will include the following (prioritized to pilots' needs):

- Support more use-cases of the Pilot Partners. Support continuous interaction with pilot partners to collect and assess feedback for improvements.
- Connection with the other two toolkits of the Suite for accessing simulation software Increase the level of complexity of the connection of DTPC with KAF.
- Prediction of success or failure as an outcome of the different process configurations.

- Improved, customizable and interactive visualizations, considering the feedback from the pilot partners.

All features are expected to be implemented by the next release of the Suite.

APPENDIX A

Nº	Comment	Action	Paragraphs
1	"However, there are few details on the implementation status. As the links in the document are directing for private sites it is hard to have a real understanding of the state of implementation. This should be corrected either by including some screenshots in the document or include links for videos in a public space."	We have added more info about the implementation in the sections "Implementation status". In the same sections we have also added screenshots and links to youtube videos. Access to GitLab repository will be given to the reviewers.	1.4.1 2.4.1 3.4.1
2	"The next developments are presented with very few details. In this regard, the preparation of a timeplan is beneficial as well as the justification for the prioritisation choices being followed in the developments"	We have added more details about future developments, prioritisation and time plan	1.4.2 2.4.2 3.4.2
3	".. as the document is only mentioning MODA, a clarification on the usage of CHADA should be made"	We have updated the document to clarify the use of MODA. CHADA is designed to document and structure data from material characterization experiments and tests, not computational modeling activities. Since our focus is on developing and defining mechanical material models rather than experimental characterization, MODA is the appropriate choice.	1.2
4	the way XAI is used should be clarified	A comment concerning XAI has been included at the document	1.4.1

Table 2: Changes in the deliverable based on the reviewers' and Project Officer's comments.